Nanoscale Disorder in Crystalline Materials

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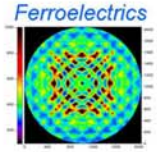
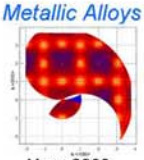
Motivation

Ferroelectrics



2005

Metallic Alloys



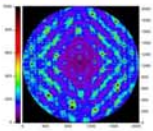
Moss 2003

Many emerging phenomena of technological importance are strongly influenced by short range correlations on the 10-100Å length scale

Molecular Solids

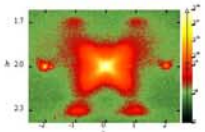
Welberry 2003

Fast Ion Conductors



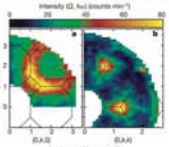
2005

CMR Oxides



Campbell 2001

Geometric Frustration



Lee 2002

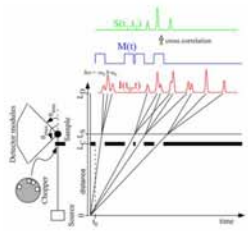
Quasicrystals

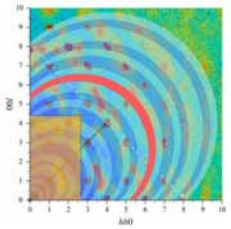
Frey 2000

- ***Develop single crystal diffuse scattering to its full potential as one of the most powerful probes of both local distortions and short range correlations***
- ***Use it in ongoing research program to study emerging complex phenomena***

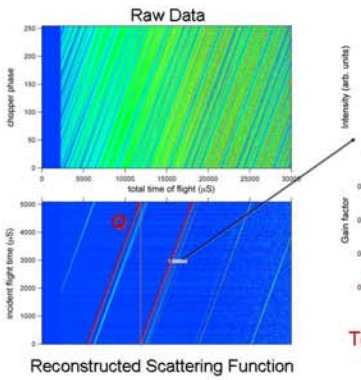
Neutron

The cross correlation method provides energy discrimination *and* efficient coverage of large volumes of reciprocal space.





- Simulations promise gains of up to a factor 100!

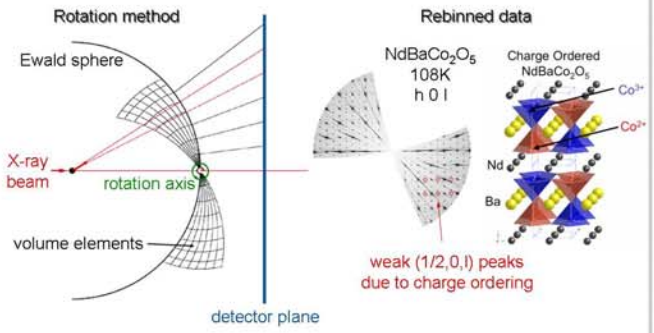


Reconstructed Scattering Function

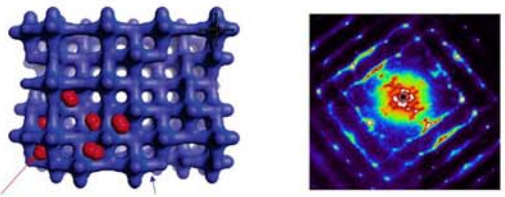
Total Gain = Gain * #Channels
~ 0.3*300

Synchrotron X-ray

- Very efficient coverage of large volumes of reciprocal space
- Simplified corrections (absorption etc) when using high energy synchrotron X-rays (> 60 keV)



- Example: diffuse scattering measured for nanoporous host-guest Prussian blue system



N_2 molecules $Mn_3[Co(CN)_6]_2$ Framework

Cross Correlation (~70) — Prototype funded (1985) — SNS Letter of Intent (2004) — Prototype design, installation (2005) — Full proposal to SNS (2006) — *Fully optimized instrument* (2007)

Workshop — High-energy X-ray rotation method — Efficient rebinning, visualization — "Ultra-fast" detectors — *Automatic refinement*

S. Rosenkranz and R. Osborn, Neutron News 15, 21 (2004)

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